Aerosol modeling with WRF/Chem

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WRF/Chem Tutorial, 31 July 2014

(Valid for WRF/Chem 3.5)

Part I - Introduction

- Overview of ...
  - Aerosol
  - Aerosol processes and life cycle
  - Model treatment of aerosol
  - WRF/Chem aerosol schemes

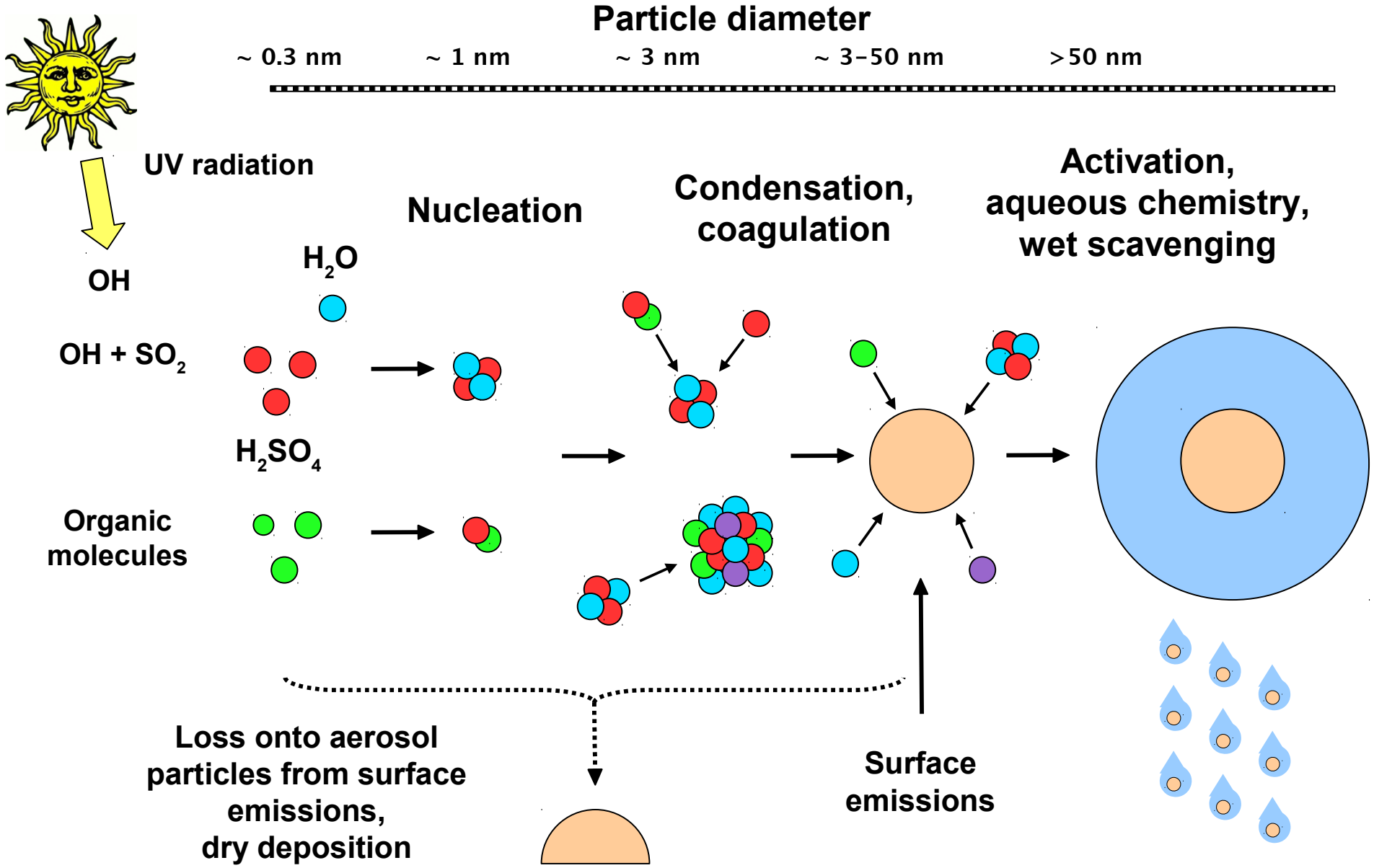
Part II – The details

- Representing the aerosol size distribution
- Walk through the WRF/Chem aerosol schemes
  - How they work and what they do
  - Coupling to other processes
    - Gas phase chemistry
    - Aqueous chemistry
    - ...
- Hint on how to tell WRF/Chem what to do
- Resources

Part I – Introduction

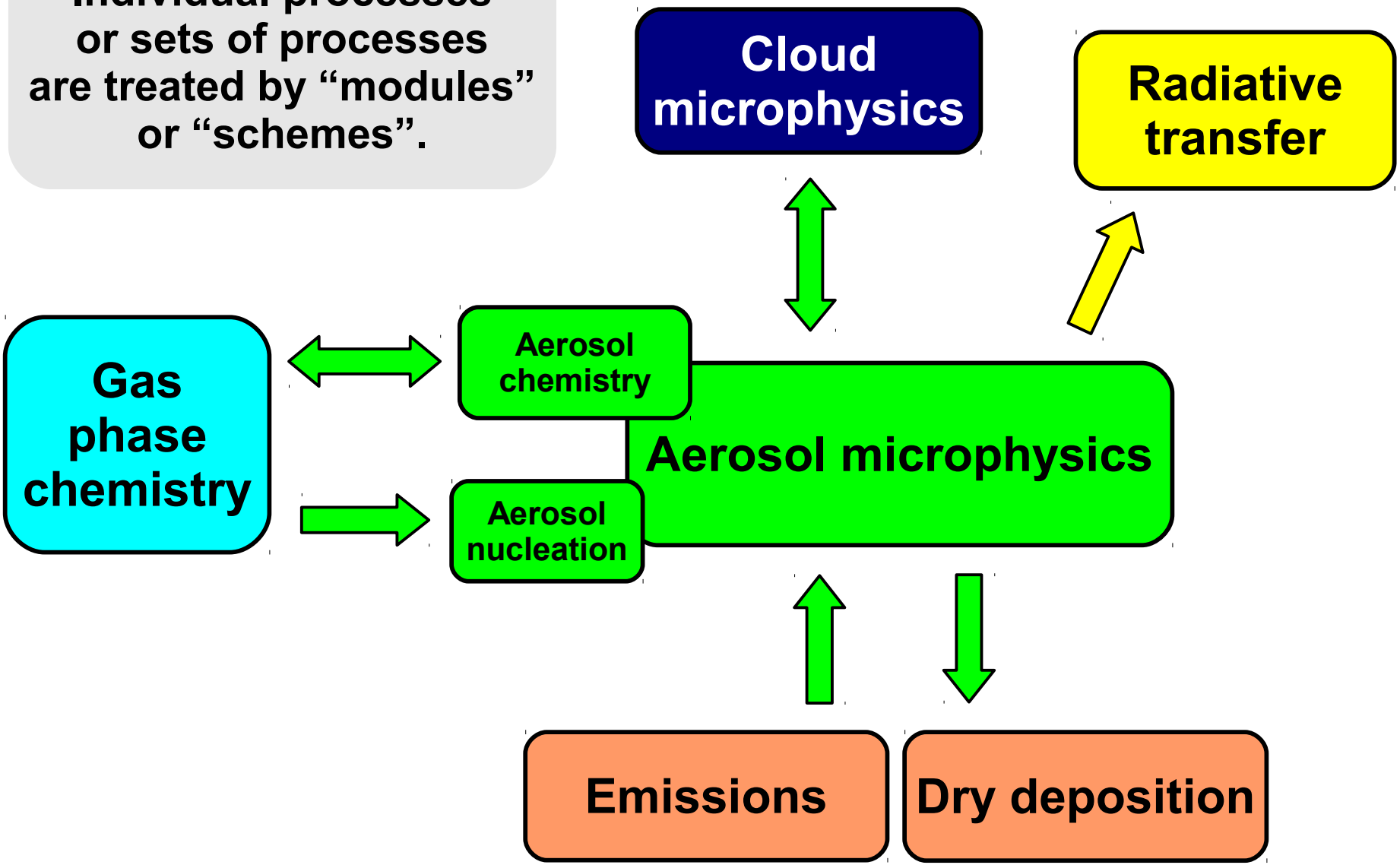
Aerosol

Aerosol life cycle and processes



Model treatment of aerosol

Individual processes or sets of processes are treated by "modules" or "schemes".



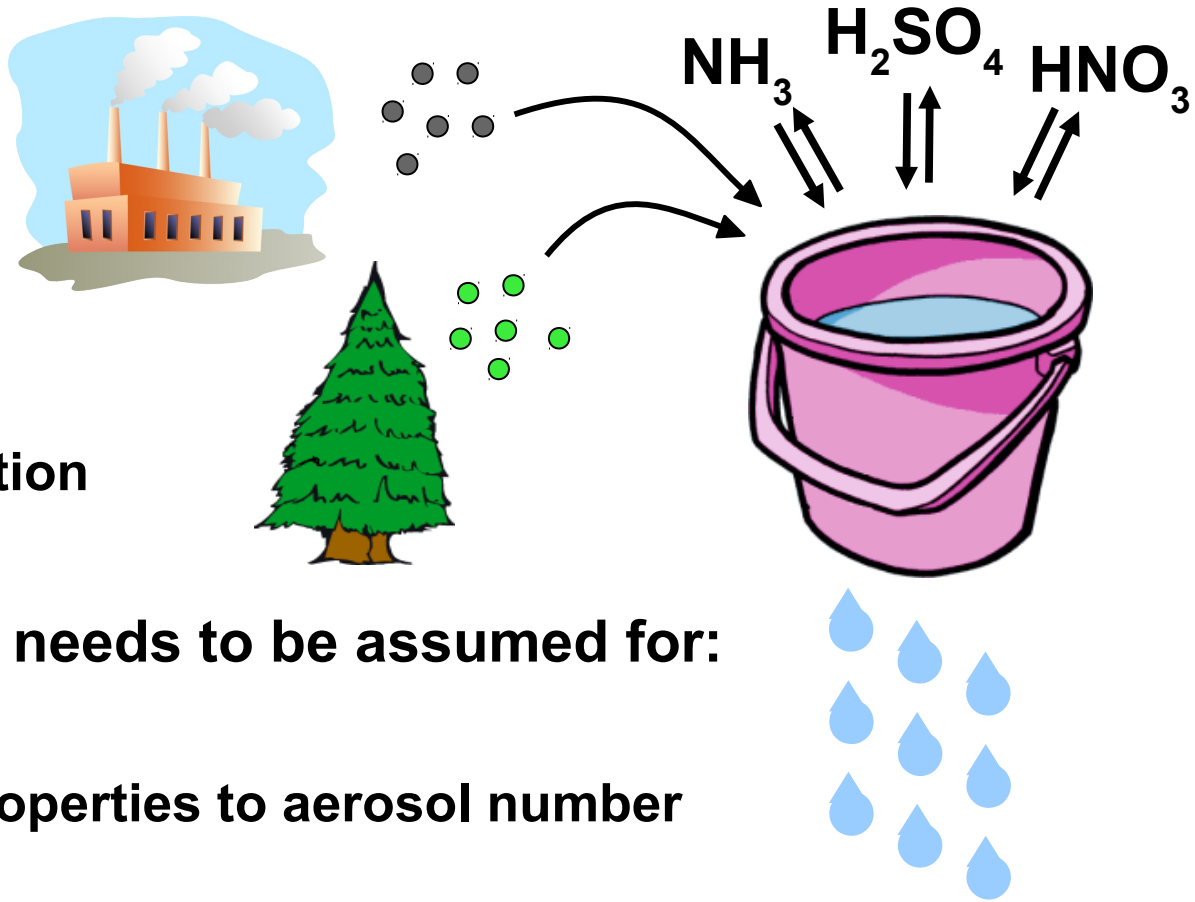
WRF/Chem aerosol schemes

- An efficient aerosol scheme from the GOCART model
  - No size information for sulfate, BC, OC
  - Size information for dust and sea salt
  - No secondary organic aerosol (SOA)
- Modal Aerosol Dynamics Model for Europe – MADE
  - 3 log-normal modes
  - Inorganic, organic aerosol, SOA
- Model for Simulating Aerosol Interactions and Chemistry (MOSAIC)
  - Sectional model, 4 or 8 bins
  - Inorganic, organic aerosol, SOA
- MAM – Modal Aerosol Model (new in WRF/Chem 3.5) from CAM5
  - 3 or 7 log-normal modes
  - Inorganic, organic aerosol, SOA, sea salt, BC, mineral dust
- Simple sectional (bin) scheme for volcanic ash aerosol

Part II – The details

Bulk aerosol schemes

- Only total mass of aerosol compounds is known



- No information on
  - Particle number
  - Aerosol size distribution

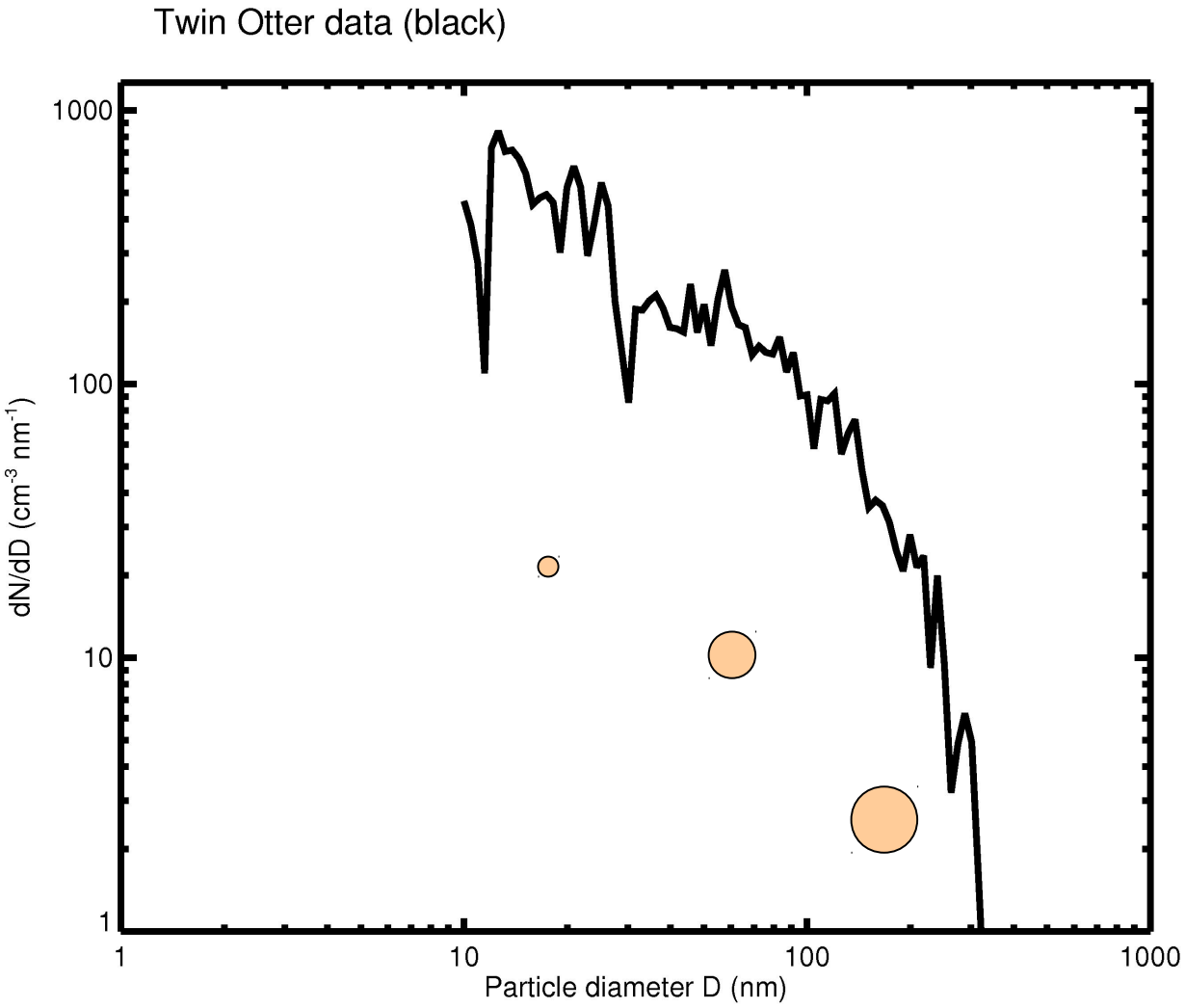
Aerosol size distribution needs to be assumed for:

- radiative transfer
- response of cloud properties to aerosol number

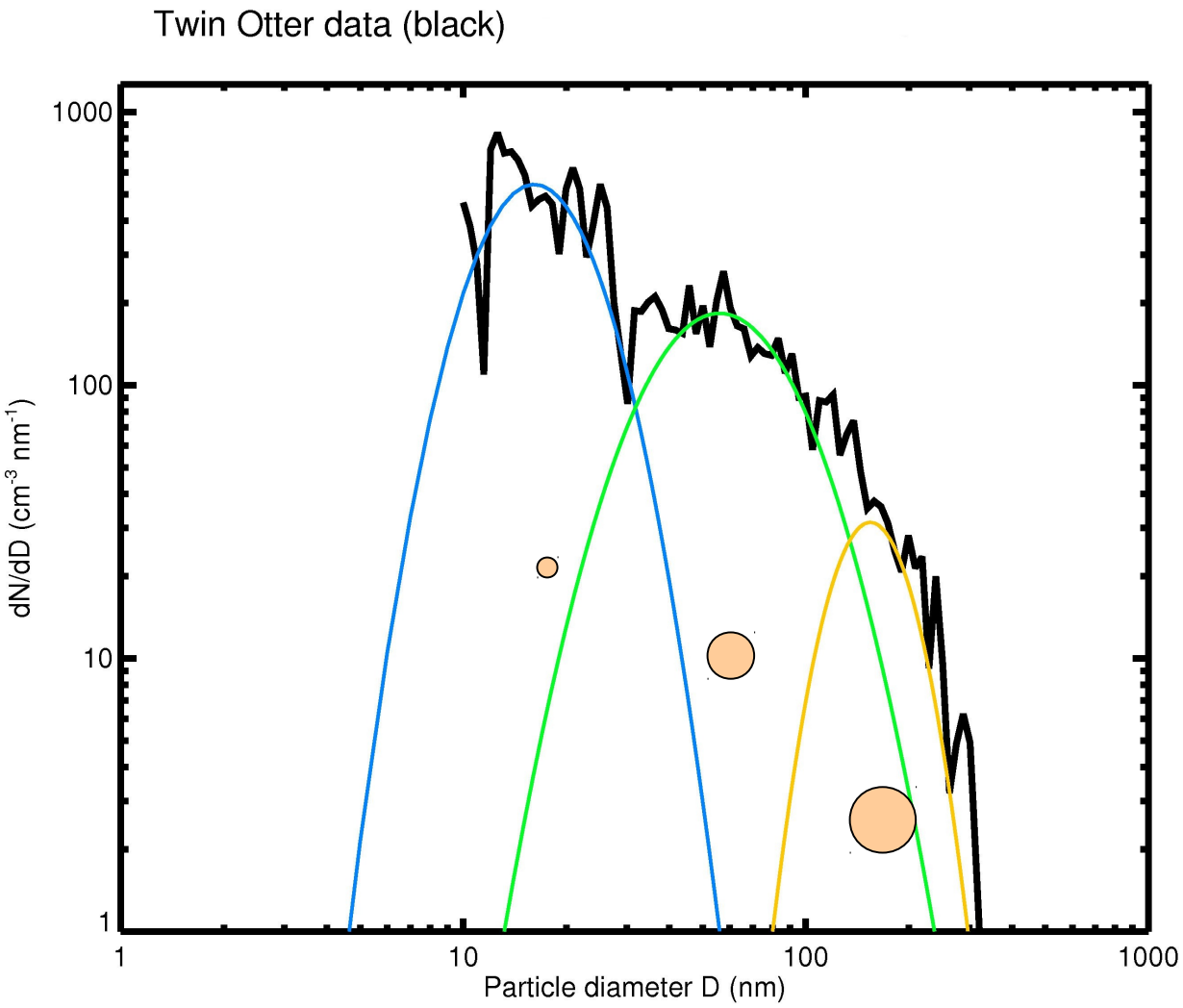
- Numerically efficient
- Useful when focus is on complex gas phase chemistry

→ GOCART (+ size resolved dust and sea salt)

Modal aerosol schemes



Modal aerosol schemes



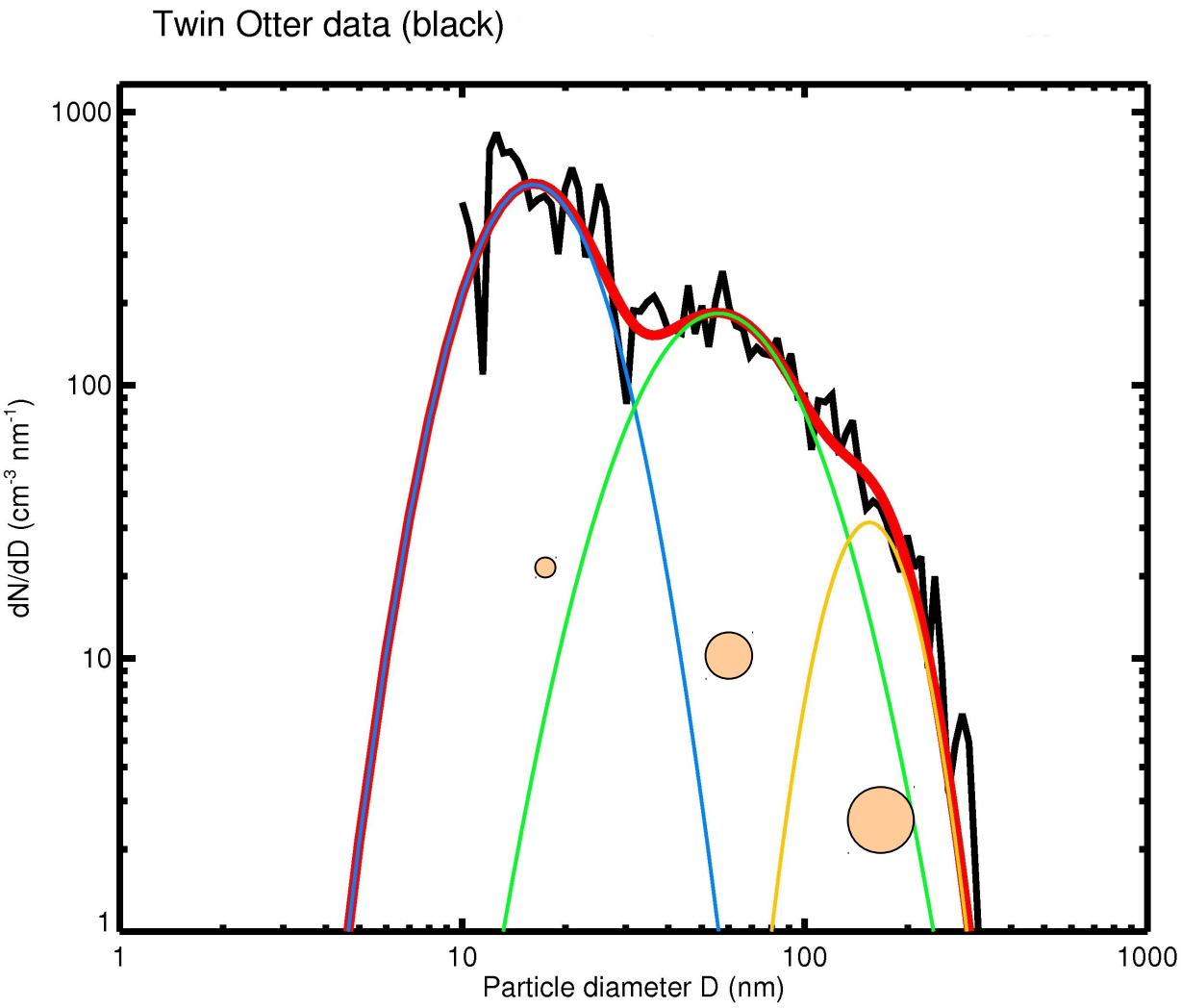
$$\frac{dN}{dD} = \frac{N}{\sqrt{2\pi}\ln(\sigma)D} e^{-\frac{1}{2}\left[\frac{\ln(D/\mu)}{\ln(\sigma)}\right]^2}$$

$\frac{dN}{dD} \rightarrow N = 8195\ cm^{-3}$
$\mu = 18.22\ nm$
$\sigma = 1.42$

$\frac{dN}{dD} \rightarrow N = 12732\ cm^{-3}$
$\mu = 68.44\ nm$
$\sigma = 1.57$

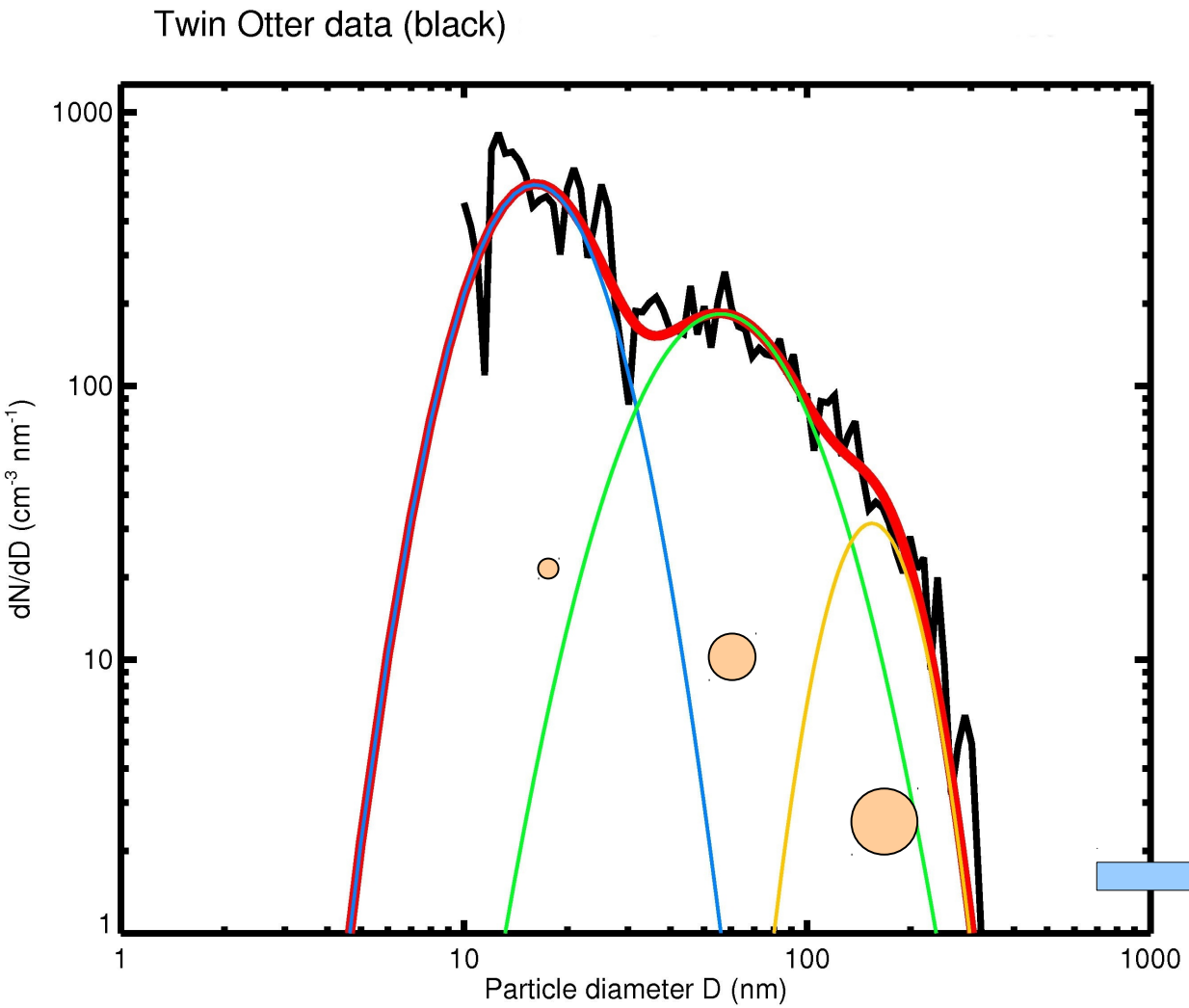
$\frac{dN}{dD} \rightarrow N = 3140\ cm^{-3}$
$\mu = 164.41\ nm$
$\sigma = 1.28$

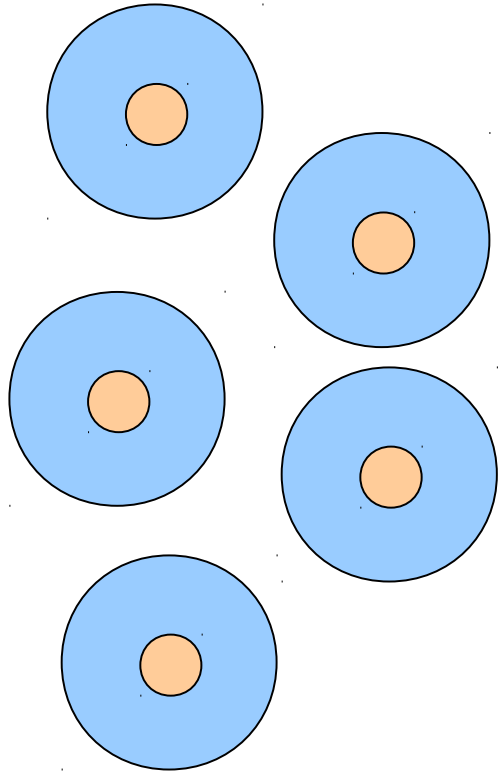
Modal aerosol schemes



$$\frac{dN}{dD} = \frac{dN}{dD} + \frac{dN}{dD} + \frac{dN}{dD}$$

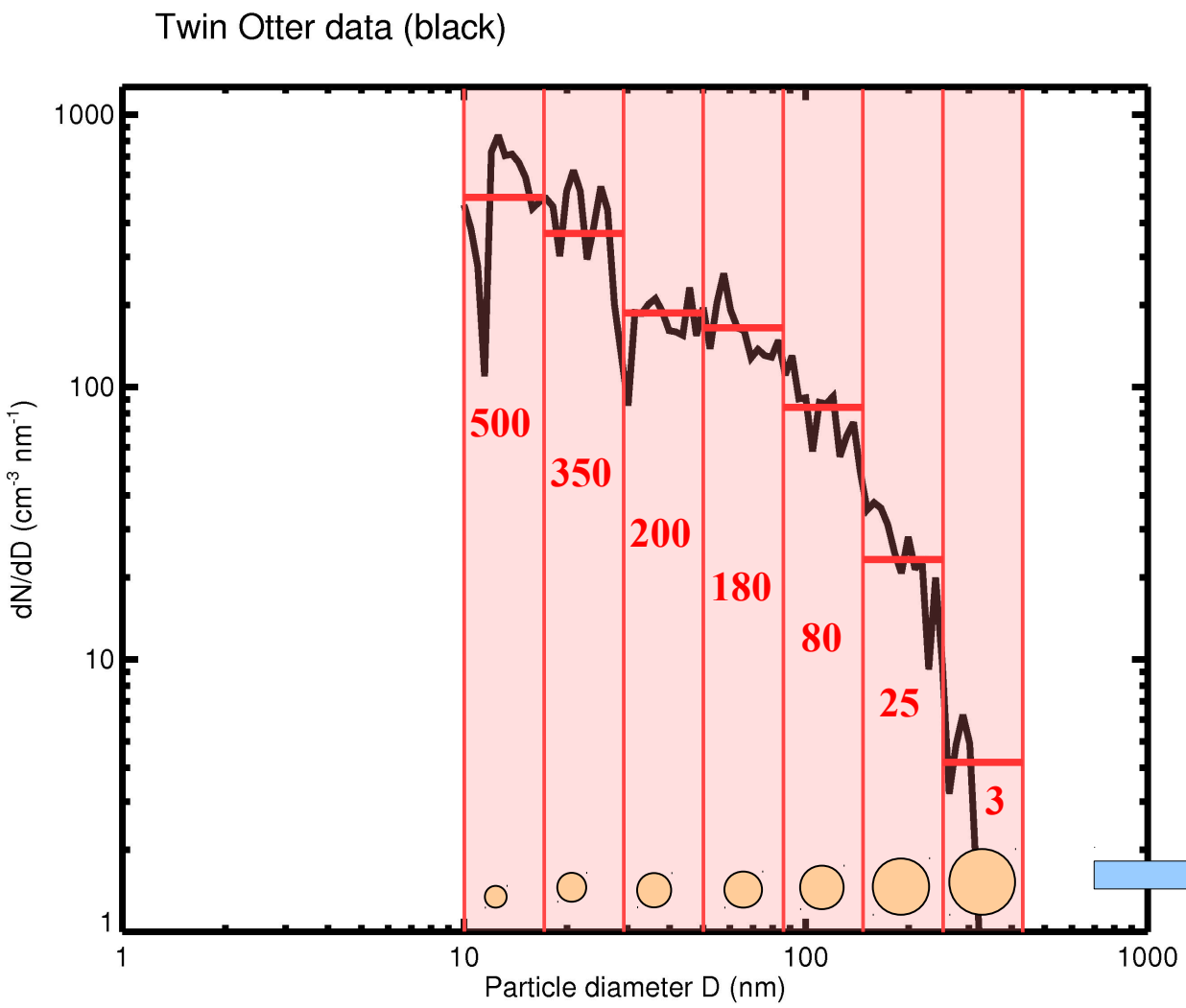
Modal aerosol schemes

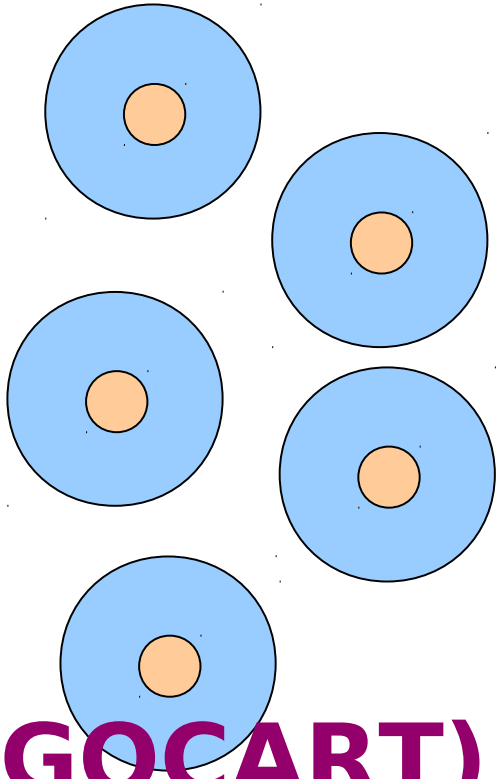




→ **MADE and MAM**

Sectional aerosol schemes





→ MOSAIC, volcanic ash, (GOCART)

GOCART aerosol module

- Georgia Tech/Goddard Global Ozone Chemistry Aerosol Radiation and Transport model (Chin et al., JGR, 2000)
  - Bulk aerosol:
    - Hydrophobic black carbon (fresh soot)
    - Hydrophilic black carbon (aged/coated soot)
    - Hydrophobic organic carbon (fresh burnt biomass)
    - Hydrophilic organic carbon (aged/coated burnt biomass)
      - Fresh → aged conversion time 2.5 days
    - Other GOCART primary PM2.5
    - Other GOCART primary PM10
    - Sulfate (only secondary aerosol species)
  - Sectional scheme for dust and sea salt:
    - Dust: 0.5, 1.4, 2.4, 4.5, 8.0 μm effective radius
    - Sea salt: 0.3, 1.0, 3.2, 7.5 μm effective radius

GOCART aerosol module

GOCART comes with sulfur gas phase chemistry:

- $DMS + OH \rightarrow SO_2 + ...$
- $DMS + OH \rightarrow MSA + ...$
- $DMS + NO_3 \rightarrow SO_2 + ...$
- $SO_2 + OH \rightarrow SO_4^{=} + ...$

Extended gas phase chemistry can be used:

- MOZART (with KPP)
- RACM (with KPP)
- RADM (with and without KPP)

GOCART aerosol module

- **Interaction with radiation:**
  - Direct effect for some model setups
  - Effect on photochemistry
- **Interaction with clouds:**
  - Aqueous chemistry
    - $SO_2 + H_2O_2 \rightarrow SO_4^=$
    - $SO_2 + O_3 \rightarrow SO_4^=$
  - No indirect effect
  - No wet scavenging/deposition
- **No secondary organic aerosol (SOA)**

MADE aerosol module

Modal Aerosol Dynamics Model for Europe

(Ackermann et al., Atm. Env., 1998)

- **3 log-normal aerosol modes: Aitken, accumulation, coarse**
- **Mode width σ is fixed**
- **Aerosol number and mass variable**
- **(Currently no nucleation mode)**
- **Interaction with radiation:**
  - **Direct aerosol effect**
  - **Effect on photolysis**
- **Interaction with clouds:**
  - **Aerosol number determines cloud drop number and size**
  - **Radiative response → 1st indirect aerosol effect**
    - **only for resolved clouds (Sc)**
  - **Aqueous chemistry**
  - **Wet removal (scavenging)**

MADE aerosol module

Aitken and accumulation modes:

- $SO_4^{=}$, NH_4^{+}, NO_3^{-}, H_2O
- NaCl (sea salt)
- Anthropogenic SOA from oxidation of ...
  - Alkanes
  - Alkenes
  - Aromatics
- Biogenic SOA from oxidation of ...
  - Alpha-pinene
  - Limonene
  - Isoprene
- Anthropogenic POA
- Elemental carbon (soot)
- Primary PM2.5

MADE aerosol module

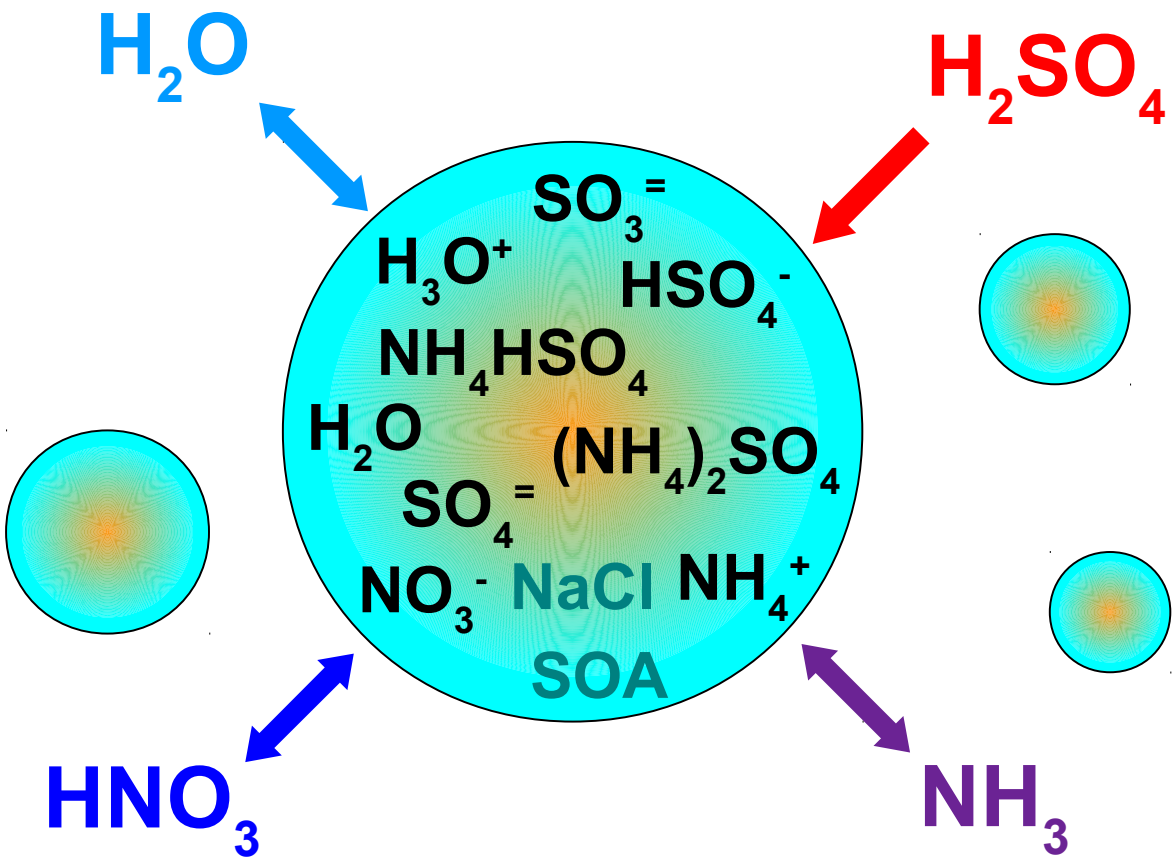
Coarse mode:

- Anthropogenic primary aerosol – e.g. from
  - Coal combustion
  - Cement manufacturing
  - Metallurgy
  - Waste incineration
- Sea salt
- Soil derived particles (mineral dust)

MADE aerosol coupling with chemistry

- **Gas phase chemistry:**
  - **RADM2 (Regional Acid Deposition Model version 2)**
  - **RACM (Regional Atmospheric Chemistry Mechanism)**
  - **RACM NOAA/ESRL version**
  - **CBMZ (Carbon-Bond Mechanism version Z)**
- **Gas phase/particle partitioning (aerosol chemistry):**
  - **MARS (Model for an Aerosol Reacting System)**
  - **SORGAM (Secondary Organic Aerosol Model)**
  - **VBS (Volatility Basis Set)**
- **Aqueous chemistry:**
  - **CMU aqueous chemistry**
  - **CMAQ (EPA) aqueous chemistry**
  - **Only for Aitken and accumulation mode**
  - **Only for selected gas phase chemistry options**

MADE and MARS: Inorganic aerosol chemistry

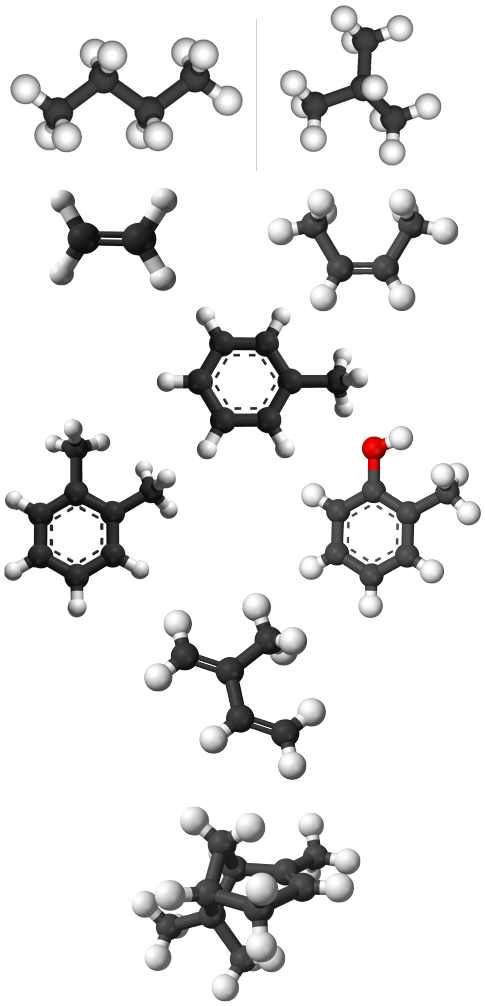


MARS (Model for an Aerosol Reacting System),
Saxena et al., Atm. Env., 1986

MADE/SORGAM

Gas phase scheme (RADM2, RACM)

- Alkanes
- Alkenes
- Toluene
- Xylene, cresole, ...
- Isoprene
- Sesquiterpene
- Alpha-pinene, limonene



OH, O_3, NO_3

Semi-volatile organics

$X_1, X_2, X_3, X_4, X_5, \ldots, X_n$

SOA

H_3O^+ HSO_4^- NH_4HSO_4 H_2O $SO_4^=$ $(NH_4)_2SO_4$ NO_3^- $SO_3^=$ NH_4^+ NaCl

SORGAM (Secondary Organic Aerosol Model), Schell et al., JGR, 2001

MADE/VBS (Volatility Basis Set)

Gas phase scheme (RACM)

Alkanes

Alkenes

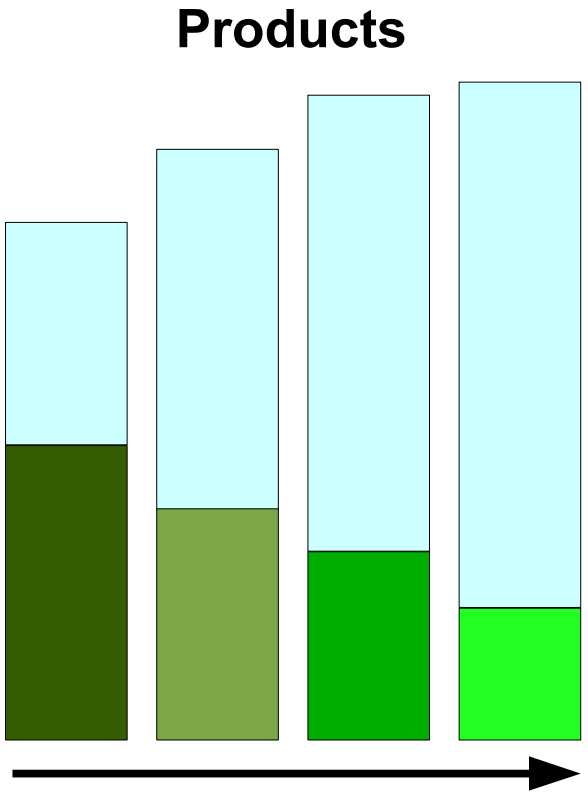
Toluene

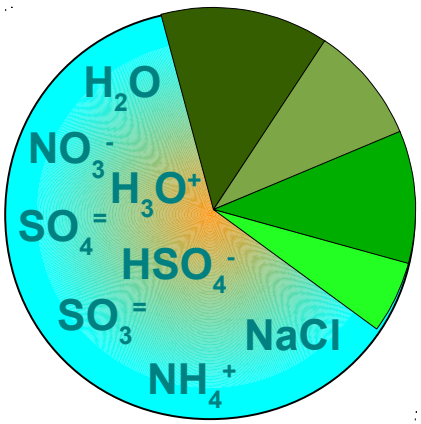
Xylene, cresole, ...

Isoprene

Sesquiterpene

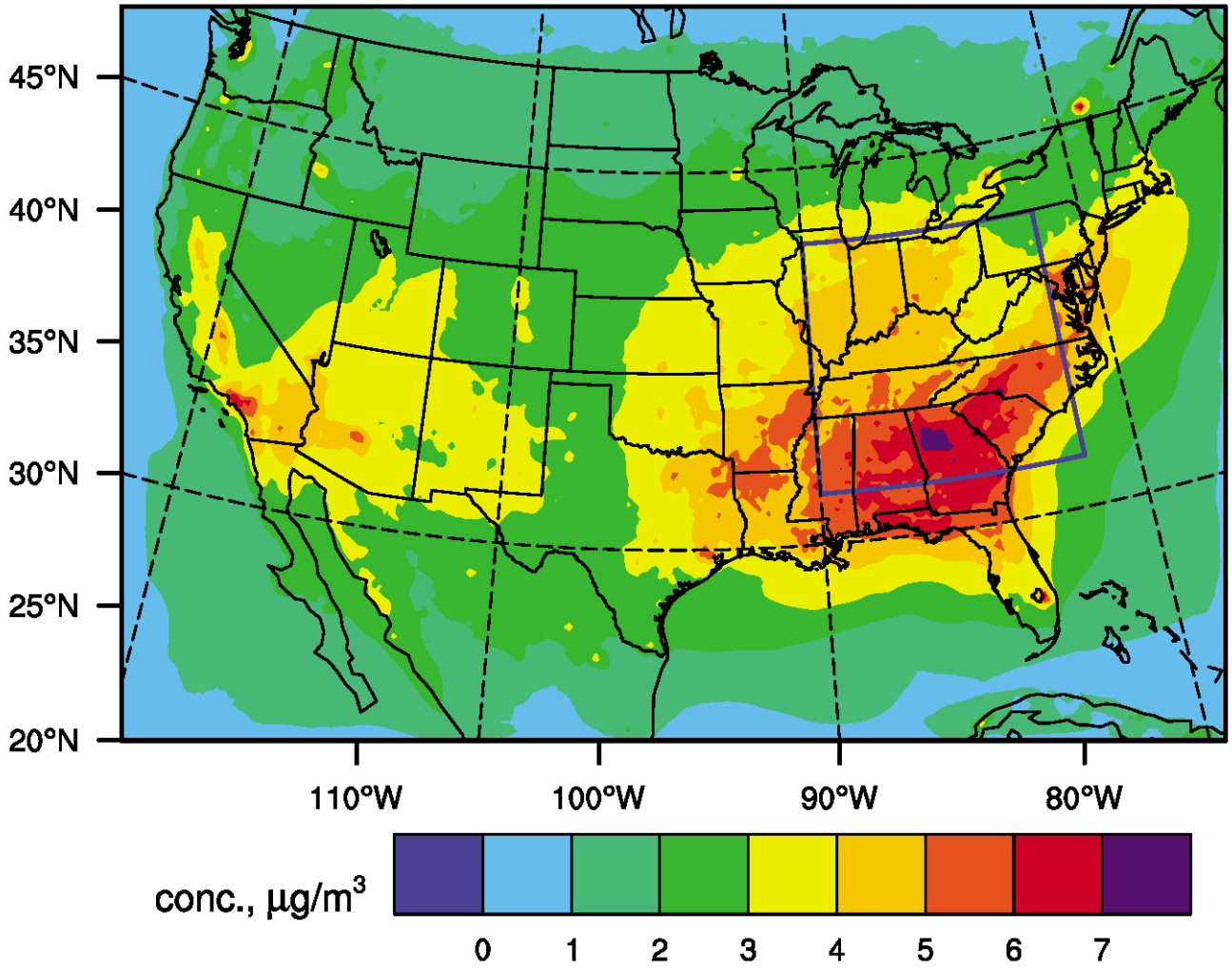
Alpha-pinene, limonene





Ahmadov et al., JGR 2012

MADE/VBS (Volatility Basis Set)



Organic aerosol mass in the surface layer (August - September 2006)

Ahmadov et al., JGR 2012

MADE and aqueous chemistry

- **CMU aqueous chemistry** (Fahey & Pandis, Atm. Env., 2001)
  - Slow
  - Only for resolved clouds (Sc)
  - Does not really conserve mass
- **CMAQ aqueous chemistry** (Walcek & Taylor, JAS, 1986)
  - Relatively fast
  - In both resolved (Sc) and parameterized (Cu) clouds
  - Coupled to wet deposition of $SO_4^=$ and NO_3^-

MADE + CMAQ aqueous chemistry

+ wet deposition of $SO_4^=$ and NO_3^- :

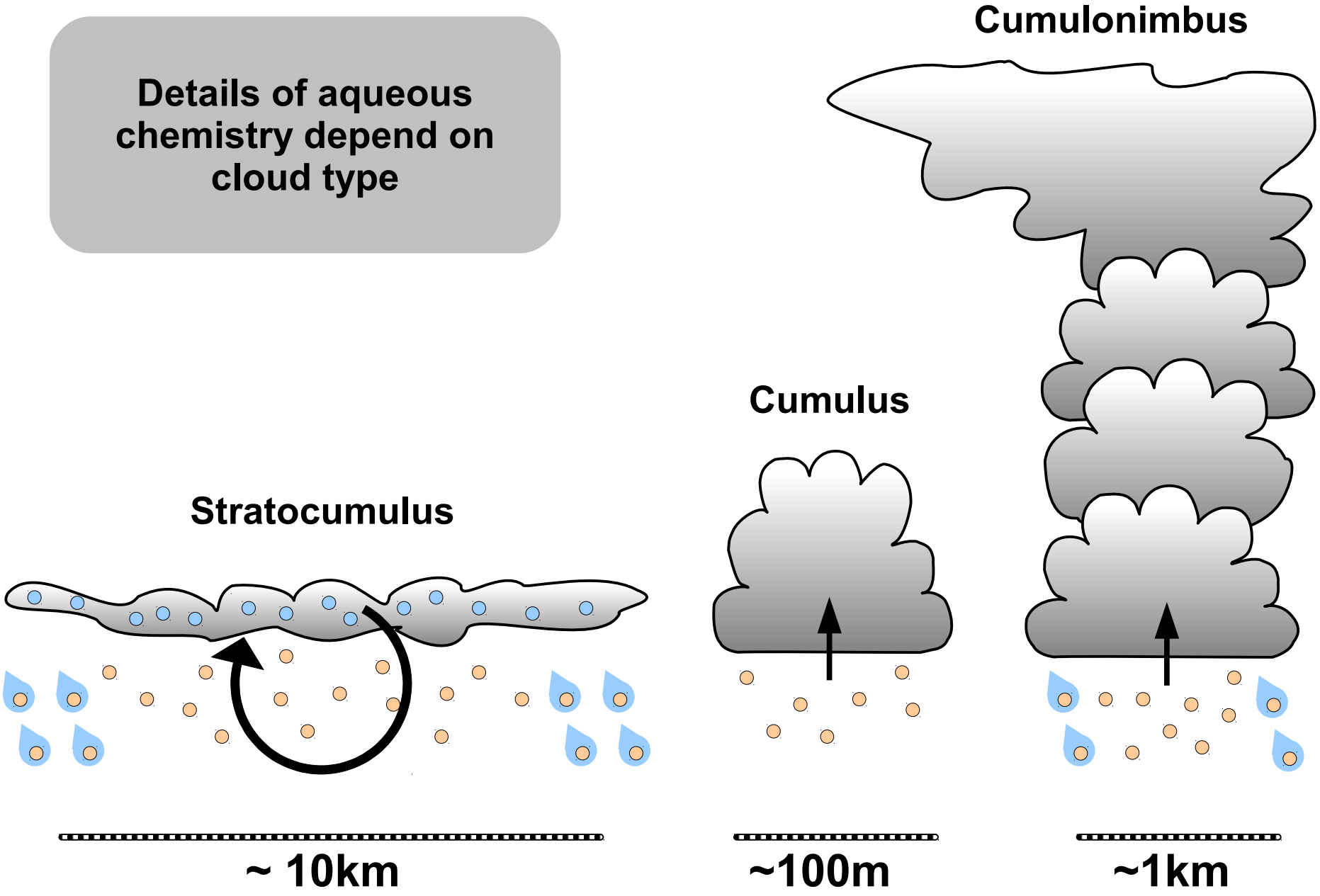
- **chem_opt = 41 : RADM2 gas phase chemistry**

Planned for WRF/Chem 3.5.1:

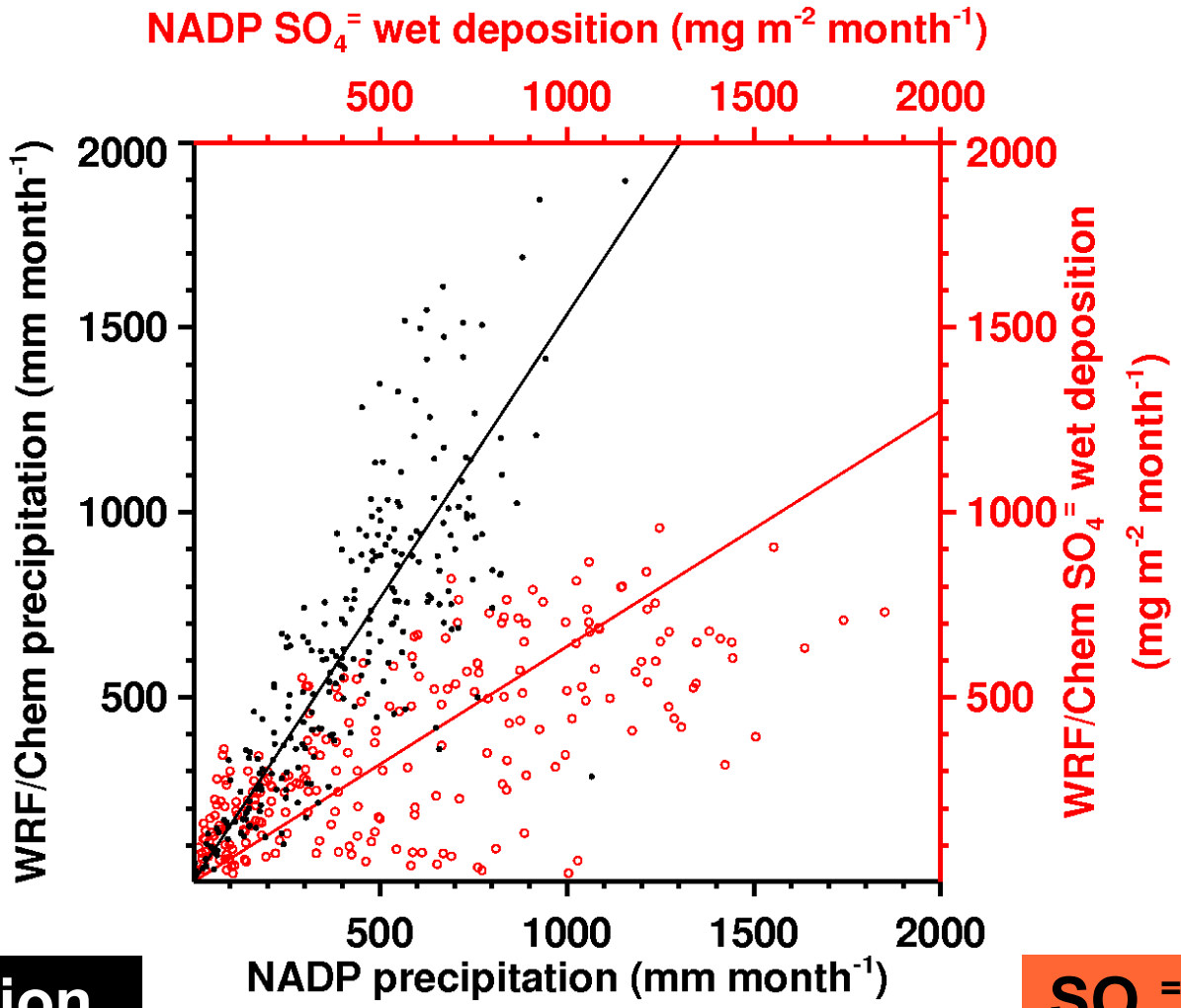
- **chem_opt = 42 : RACM gas phase chemistry (KPP)**
- **chem_opt = 43 : RACM ESRL gas phase chemistry (KPP)**

MADE and CMAQ aqueous chemistry

Details of aqueous chemistry depend on cloud type



MADE and wet deposition



Precipitation	
r	model/obs.
0.81	1.25

$SO_4^=$ wet dep.	
r	model/obs.
0.86	0.53

May-September 2006
(National Atmospheric Deposition Program)

MOSAIC aerosol module

Model for Simulating Aerosol Interactions and Chemistry (Zaveri et al., JGR, 2008)

- Modern aerosol scheme in WRF/Chem
- 4 or 8 aerosol size sections (bins) 39 nm – 10 μm
- (Lower bin boundary of 39 nm too large for nucleation)
- Interaction with radiation:
  - Direct aerosol effect
  - Effect on photolysis
- Interaction with clouds:
  - Aerosol number determines cloud drop number and size
  - Radiative response → 1st indirect aerosol effect
  - Aqueous chemistry
  - Wet removal (scavenging)
  - only for resolved clouds (Sc)

MOSAIC aerosol module

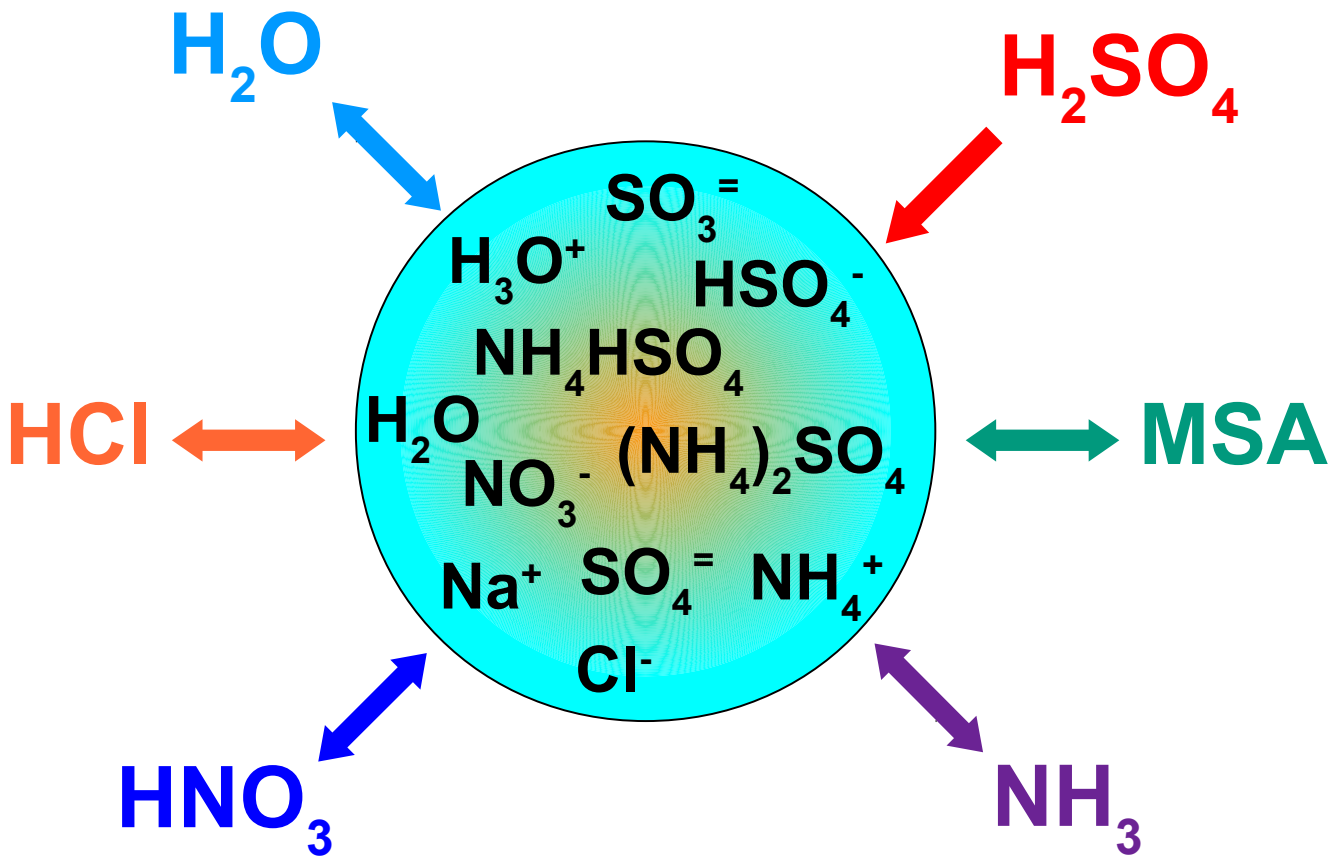
Aerosol composition

- $SO_4^{=}$, NH_4^{+}, NO_3^{-}, H_2O
- NaCl (sea salt)
- CH_3SO_3 (methanesulfonate)
- carbonate (CO_3)
- calcium (Ca)
- black carbon (BC)
- primary organic mass (OC)
- other inorganic mass (minerals, trace metals)

MOSAIC aerosol coupling with chemistry

- **Gas phase chemistry:**
  - **CBMZ (Carbon-Bond Mechanism version Z)**
    - "Standard" gas phase chemical scheme for MOSAIC
  - **SAPRC99 (extensive VOC chemistry)**
    - Works with the VBS SOA scheme
  - **MOZART (Model for Ozone and Related chem. Tracers)**
    - Works with the VBS SOA scheme
- **Gas phase/particle partitioning (aerosol chemistry):**
  - **MTEM (Multicomponent Taylor Expansion Method)**
  - **MESA (Multicomponent Equilibrium Solver for Aerosols)**
  - **VBS (Volatility Basis Set)**
- **Aqueous chemistry:**
  - **CMU aqueous chemistry, only for resolved clouds (Sc)**
  - **Not with KPP versions of gas phase chemistry schemes**

MOSAIC, MTEM, and MESA



MTEM calculates activity coefficients
MESA solves ion-equilibria in the liquid phase
For SOA: VBS (Volatility Basis Set) scheme

MTEM (Multicomponent Taylor Expansion Method), Zaveri et al., JGR 2005a
MESA (Multicomponent Equilibrium Solver for Aerosols), Zaveri et al., JGR 2005b

MAM aerosol module

Modal Aerosol Model from CAM5

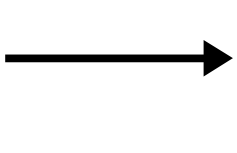
- New in WRF/Chem 3.5
- 3 or 7 log-normal aerosol modes: MAM3 and MAM7
- Mode width σ is fixed
- Aerosol number and mass variable
- Liu et al., Geosci. Model Dev., 5, 709-739, 2012

MAM 3

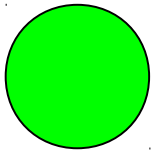
Aitken mode

- Sulfate ($SO_4^=$)
- SOA
- Sea salt

Coagulation, condensation

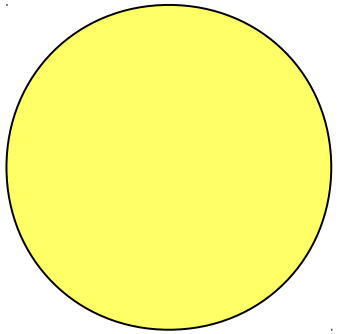


Accumulation mode



- Sulfate ($SO_4^=$)
- SOA
- Primary organic matter
- Sea salt
- Black carbon
- Mineral dust
- Sea salt

Coarse mode



- Sulfate ($SO_4^=$)
- Mineral dust
- Sea salt

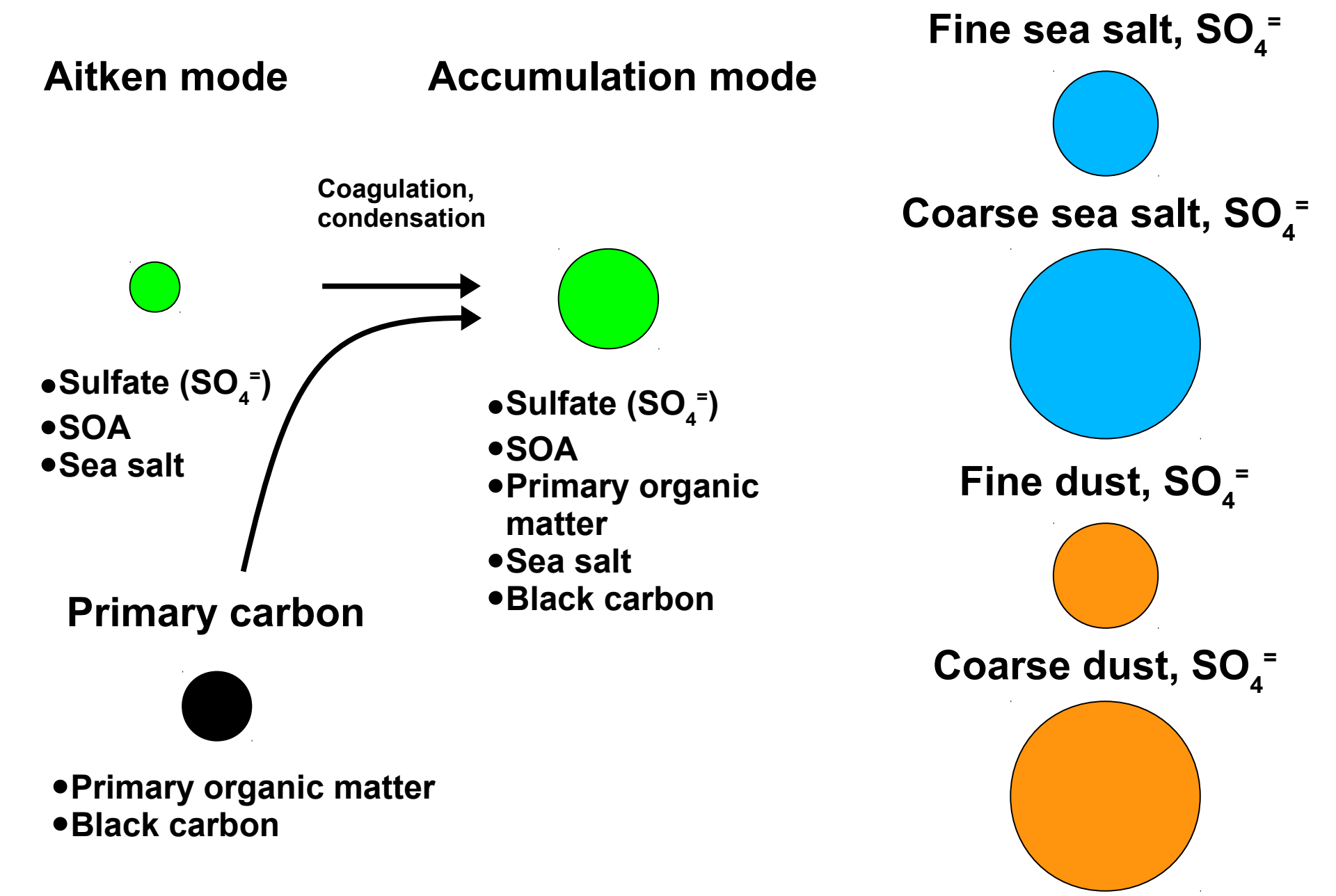
15 – 53 nm

58 – 270 nm

0.8 – 3.65 µm

Dry particle diameter

MAM 7


Aitken mode
Accumulation mode
Coagulation, condensation
•Sulfate ($SO_4^=$)
•SOA
•Sea salt
•Sulfate ($SO_4^=$)
•SOA
•Primary organic matter
•Sea salt
•Black carbon
Primary carbon
•Primary organic matter
•Black carbon
Fine sea salt, $SO_4^=$
Coarse sea salt, $SO_4^=$
Fine dust, $SO_4^=$
Coarse dust, $SO_4^=$

MAM aerosol module

- **Currently only one gas phase chemistry scheme**
  - **CBMZ (Carbon-Bond Mechanism version Z)**
- **Interaction with radiation:**
  - **Coupled to RRTMG radiation → Direct aerosol effect**

As in CAM5:

- **Gas phase/particle partitioning (aerosol chemistry):**
  - **Condensation of water vapor and of the 4 inorganic trace gase species: NH_3, H_2SO_4, HNO_3, HCl**
- **Interaction with clouds only resolved clouds (Sc):**
  - **Coupled to Morrison & Gettelman cloud microphysics**
  - **Radiative response → 1st indirect aerosol effect**
  - **Wet removal (scavenging)**
  - **Aqueous chemistry**
- **Dry deposition**

Volcanic ash

- 10 bins for volcanic ash aerosol
- Transport, settling, dry deposition
- Currently no other aerosol
- Single active volcano
- Database of 1535 volcanoes (latitude, longitude, height)

How to tell WRF/Chem what to do

../WRFV3/test/em_real/real.exe
../WRFV3/test/em_real/namelist.input
../WRFV3/test/em_real/...
../WRFV3/test/em_real/...

```
  ...
  ...
 &chem
 chem_opt         = 42
 photdt           = 0.25
 chemdt           = 0
  ...
aerchem_onoff     = 1
  ...
conv_tr_aqchem    = 1
```

MADE/SORGAM, RACM, CMAQ aqueous chemistry

Switches all aerosol processes on/off

CMAQ aqueous chemistry on in Cu

Resources

- WRF/Chem User's Guide
  - Model options (namelist parameters)
  - Combinations of physical/chemical schemes
  - ...
- Papers referenced in the WRF/Chem User's Guide
- WRF/Chem source code

- WRF/Chem Help (wrfchemhelp.gsd@noaa.gov)
- Yours truly (jan.kazil@noaa.gov)